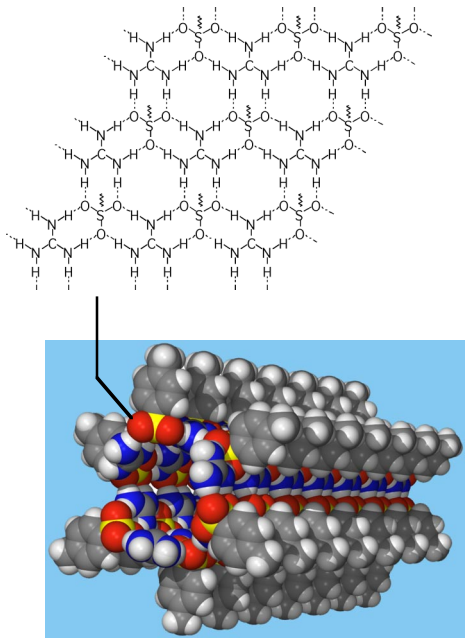
Functional Organic Solid State Materials Derived from Designer Host Frameworks

DMR-0305278

Michael D. Ward, University of Minnesota

guanidinium-sulfonate sheet



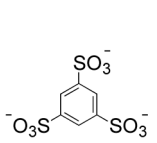
"van der Waals tube"

Horner, et al., *Angewandte Chemie,* 40, 4045 (2001)

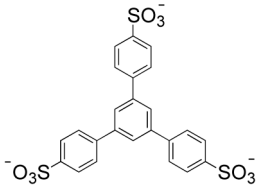
- Previously demonstrated that hydrogen-bonded nanotubes, formed by guanidinium-sulfonate sheets curved into continuous surfaces, assemble into crystals through non-covalent van der Waal interactions between organic groups projecting from outer tube surface
- Formation of nanotubes must compete with formation of layered structures, the selectivity depending on the identity of the organic substituent appended to the sulfonate and the templating guest (which is needed for tube formation)

Fall 2003

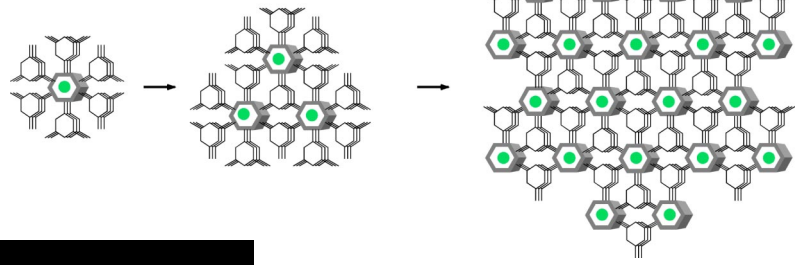
Strategy: Use polytopic sulfonates to prohibit formation of layered phases and promote formation of tesselated networks of tubes through topological complementarity

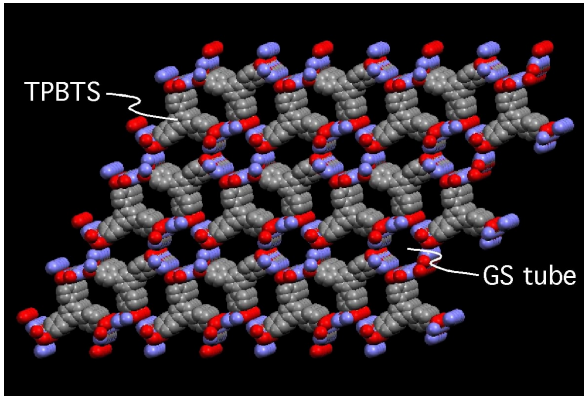


BTS



TPBTS





A tesselated guanidinium-sulfonate tube network with TPBTS (guest molecules omitted for clarity)

S.-J. Park, M. A. Horner, M. D. Ward, *in progress*

- The BTS and TPBTS trianions, both with 3-fold symmetry that complements the hexagonal symmetry of the guanidinium-sulfonate tube, promote formation of tesselated tube networks in which each tube is connected through *covalent* linkers while prohibited the formation of competitor layered structures
- A rare example of true crystal design and synthesis
- Work in progress: (*i*) explore whether guest molecules are needed to form tubes, (*ii*) explore whether covalent tesselation prevents collapse of tubes when guests are removed, (*iii*) explore whether the trianions promote tube formation for guests that do not induce formation of van der Waals tubes, (*iv*) explore the influence of intertube spacing on interchannel ordering of polar and paramagnetic guests

Broader Impact Y2002 - 2003

Michael D. Ward, University of Minnesota

Education and Mentoring

- 4 Graduate students related to project: Matt Horner, Steve Martin, David Plaut (now at 3M), Sang-Jae Park
- 1 Postdoc:Sang-Ok Park
- 2 Undergraduates performing laboratory research: Amelia Anderson (guest student from Clemson REU), John Maciejewski (UMN MRSEC REU student from Penn State)
- Organized and hosted the *Midwest Organic Solid State Chemistry Symposium* (MOSSCS XIV), a two-day symposium attended by nearly 100 students from Midwest and some East Coast universities, with an emphasis on presentations by graduate students and postdoctoral associates
- Host for Taesung Jung, a visiting student (one year appointment) from Seoul National University supported entirely by the Korea Ministry of Education through the Brain Korea-21 program

Outreach

- Activities revolving around role as director of the University of Minnesota MRSEC (tribal college visits, overseeing overall operation of MRSEC-related outreach programs, including visiting faculty-student teams and individual undergraduates during summer 2003.

Industrial connections

- Eli Lilly

International and other Activities

- Associate Editor, Chemistry of Materials
- Director, University of Minnesota MRSEC
- Concluded initial phase of grazing incidence X-ray diffraction studies at the DESY synchotron facility (Hamburg, Germany) with co-workers from the Weizmann Institute (*J. Am. Chem. Soc.*, in press)
- One of two UMN representatives at the Brain Korea -21 International Symposium at Seoul National University (serving to fortify research collaboration and student exchange between the two institutions)